An analytic kinetic approach to Zener interminiband transitions in superlattices

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Abstract. Starting from an equation-of-motion analysis of the density matrix, phenomenological kinetic equations are derived that allow a study of semiclassical intraband and quantum-mechanical tunneling contributions to the current densities. An analytical expression is obtained, which describes the field dependence of the electron densities in the upper and lower minibands. It is shown that a population inversion does not occur as long as the scattering time for thermal generation is larger than the interminiband relaxation time. Numerical results for the current density are discussed.

1. Introduction

Recently, there have been intensive investigations of the influence of external electric fields on semiconductor superlattices (SLs). The physics of biased SLs is extremely rich due to the large number of parameters that can be controlled quite independently. Most of the interest has been caused by the need of understanding the interplay of Bloch oscillations, Zener tunneling between Bloch bands, and interaction effects. From a theoretical point of view the simplest models involve only a single miniband. This approach leaves out all interesting interminiband phenomena, which are captured most simply in a two-band tight-binding model. The purpose of the present work is to study the nonequilibrium carrier kinetics by an equation-of-motion analysis of the density matrix and a derivation of an expression for the current, from which semiclassical intraband and quantum-mechanical tunneling contributions can be identified. Starting from a microscopic theory, we derive phenomenological kinetic equations by using the constant relaxation-time approximation. The dynamics of electrons is treated in a simple two-band SL model. Former theoretical studies [,] of unipolar devices will be extended by taking into account all relevant horizontal and vertical electron transitions. In addition, the widely used Esaki–Tsu model [ ] is extended to two-band systems.

2. Theoretical model

The quantum-kinetic equation for the Wigner transformed elements of the density matrix $f_\nu^{\nu'}(k)$ (with ν, ν' being miniband indices), whose explicit spatial dependence describing field domains is not taken into account, is given by [ ]

$$\left\{ \frac{e}{\hbar} E \nabla_k + \frac{i}{\hbar} [\varepsilon_{\nu'}(k) - \varepsilon_\nu(k)] \right\} f_\nu^{\nu'}(k) \tag{1}$$

$$+ \frac{ieE}{\hbar} \sum_\mu \left[Q_{\mu\nu}(k) f_\mu^{\nu'}(k) - Q_{\nu'\mu}(k) f_\nu^\mu(k) \right] = \sum_{\mu\mu'} \sum_{k_1} f_\mu^{\mu'}(k_1) W_{\mu\nu}^{\mu'\nu'}(k_1, k),$$
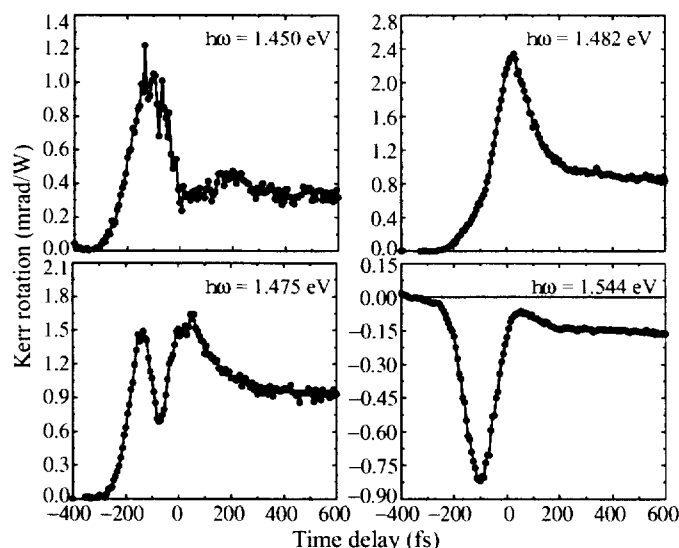
Fig. 2. The dynamical Kerr rotation spectra as a function of time delay in the femtosecond time domain.

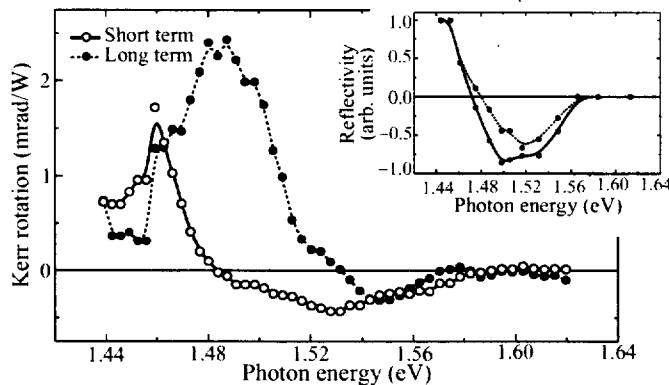**Fig. 3.** The spectral dependence of the induced Kerr rotation for two delay times $t = 0$ and $t = 500$ fs.

Acknowledgements

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where the matrix elements

$$Q_{\mu\mu'}(k) = \sum_K \chi_{\mu'}(k + K)\nabla_{k_z}\chi_\mu^*(k + K) \tag{2}$$

determine the wavefunction overlap calculated from the SL envelope functions χ_μ. The Q-term in Eq. (1) describes electric-field-induced vertical transitions via Zener tunneling. We consider a two-band model characterized by the tight-binding minibands

$$\varepsilon_1(k) = \frac{\hbar^2 k_\perp^2}{2m} + \frac{\Delta_1}{2}(1 - \cos k_z d), \tag{3}$$

$$\varepsilon_2(k) = \frac{\hbar^2 k_\perp^2}{2m} + \varepsilon_g + \Delta_1 + \frac{\Delta_2}{2}(1 + \cos k_z d). \tag{4}$$

Δ_1 (Δ_2) is the bandwidth of the lower (upper) miniband, and ε_g the energy gap between the minibands. $k_\perp$ is the quasi-momentum of the lateral electron motion. To lowest order in the coupling constant, only the transition probabilities W_{11}^{11}, W_{22}^{22}, W_{12}^{12}, W_{21}^{21}, W_{22}^{11}, and W_{11}^{22} have to be accounted for. We will study the kinetic equation (1) in the constant relaxation time approximation by making use of the replacement

$$\mathrm{Re}\,W_{22}^{11}(k', k) = \mathrm{Re}\,W_{11}^{22}(k', k) \rightarrow -\delta_{k'k}/\tau \tag{5}$$

for the interminiband transition probabilities. The horizontal interminiband transitions via thermic generation W_{12}^{12} and recombination W_{21}^{21} are described by relaxation times τ_1' and τ_2', respectively. Finally, for the description of intraminiband transitions, we use the extended Esaki–Tsu model [ ]. Focusing on high electric fields, where $\Omega > 1/\tau_{\mathrm{eff}}$ ($\Omega = eEd/\hbar$ is the Bloch frequency and τ_{eff} an effective scattering time), and taking into account the periodicity of $f_\nu^{\nu'}(k)$ along the field direction k_z, we switch to the Wannier–Stark representation by Fourier transforming the distribution function [ ]

$$f_\nu^{\nu'}(k) = \sum_{l=-\infty}^{\infty} e^{ilk_z d} f_\nu^{\nu'}(k_\perp, l). \tag{6}$$

We neglect the smooth k_z dependence in $Q_{\mu\mu'}(k_z)$ and obtain the following analytical result for the electron density n_2 of the upper miniband

$$n_2 = \frac{2(\Omega\tau)^2 A_0 + \tau/\tau_1'}{4(\Omega\tau)^2 A_0 + \tau/\tau_1' + \tau/\tau_2'}, \quad A_0 = \sum_{l\neq 0} \frac{q(l)^2}{(l\Omega\tau - \Omega_g\tau)^2 + 1}. \tag{7}$$

In the expression for A_0, we introduced the abbreviations

$$q(l) = (-1)^l Q_{12} J_l\left(\frac{\Delta_1 + \Delta_2}{2\hbar\Omega}\right), \quad \Omega_g = \frac{\varepsilon_g + (\Delta_1 + \Delta_2)/2}{\hbar} - \Omega(Q_{22} - Q_{11}). \tag{8}$$

with J_l denoting the Bessel function. In the absence of thermal generation $\tau_1' \rightarrow \infty$ and under the condition $n_2 \ll 1$, we recover the result $n_2 \approx 2\Omega^2\tau\tau_2' A_0$ derived already in [ ]. From Eq. (7), it is seen that population inversion occurs only under the unrealistic condition $\tau_2' > \tau_1'$ independently of the value of the electric field strength.
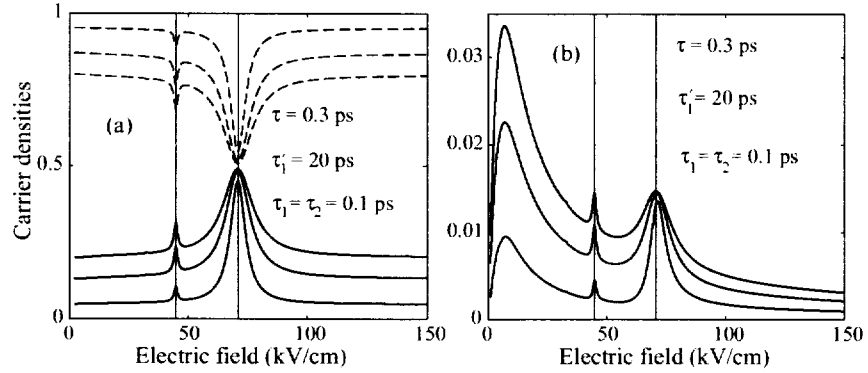
Fig. 1. (a) Electric-field dependence of the carrier density for the upper (solid lines) and lower (dashed lines) minibands. The bandwidth of the lower (upper) miniband is $\Delta_1 = 5$ meV ($\Delta_2 = 40$ meV). The two minibands are separated by an energy gap of $\varepsilon_g = 100$ meV and the temperature is $T = 300$ K. We use identical intraminiband relaxation times $\tau_1 = \tau_2 = 0.1$ ps and the following values for the interminiband scattering times $\tau = 0.3$ ps and $\tau_1' = 20$ ps. For the solid curves from bottom to top, the interminiband recombination time τ_2' is given by 1, 3, and 5 ps. The positions of Zener resonances at $l\Omega = \Omega_g$ ($l = 1, 2$) are marked by thin vertical lines.
(b) The same as in (a) for the relative current density j_z/j_0 with $j_0 = en_s(\Delta_1 + \Delta_2)/2\hbar$. n_s is the carrier sheet density.

An analytical expression for the current density is obtained from [ ]

$$
j_z = -\frac{n}{E} \sum_{kk'} \left\{ \varepsilon_1(k_z) f_1^1(k') W_{11}^{11}(k', k) + \varepsilon_2(k_z) f_2^2(k') W_{22}^{22}(k', k) \right.
$$
$$
\left. + \varepsilon_1(k_z) f_2^2(k') W_{21}^{21}(k', k) + \varepsilon_2(k_z) f_1^1(k') W_{12}^{12}(k', k) \right\},
\tag{9}
$$

where n denotes the total electron density.

3. Numerical results and discussion

Numerical results for the carrier densities and the relative current j_z/j_0 are shown in Fig. 1(a) and (b). The set of parameters used in the calculation is given in the caption. The matrix elements $Q_{\mu\mu'}$ have been estimated with wavefunctions of a quantum well with infinite potential barriers. A characteristic feature in these graphs is the appearance of Zener resonances at $l\Omega = \Omega_g$, which are shifted to larger field strengths with increasing energy gap ε_g so that at low electric fields the well-known Esaki–Tsu current-voltage characteristics [ ] is recovered. The lineshape of the Zener resonances depends sensitively on the miniband widths. Whereas the carrier density n_2 is a function of the sum $\Delta_1 + \Delta_2$, pronounced current resonances occur only for narrow lower and broad upper minibands. With increasing interminiband relaxation time τ the peaks become sharper. When the generation and recombination lifetimes are identical ($\tau_1' = \tau_2'$), we obtain from Eq. (7) $n_2 = 0.5$ independently of the electric field strength. As long as thermal generation can be neglected ($\tau_2' < \tau_1'$), a population inversion cannot occur in the considered SL model.

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